Ridge Regression

Nipun Batra

IIT Gandhinagar

August 1, 2025

Introduction

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In $f(x) = c_0 + c_1 x + c_2 x^2 + \dots$ it is $\max |c_i|$

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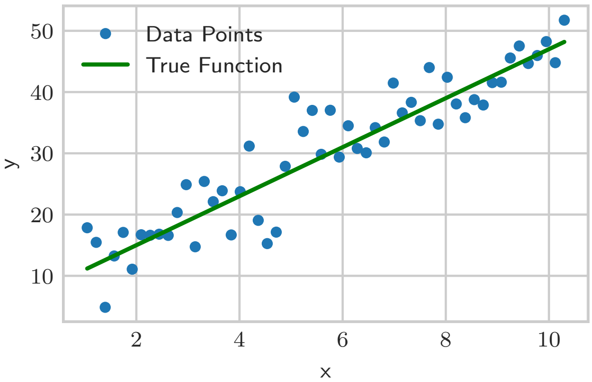
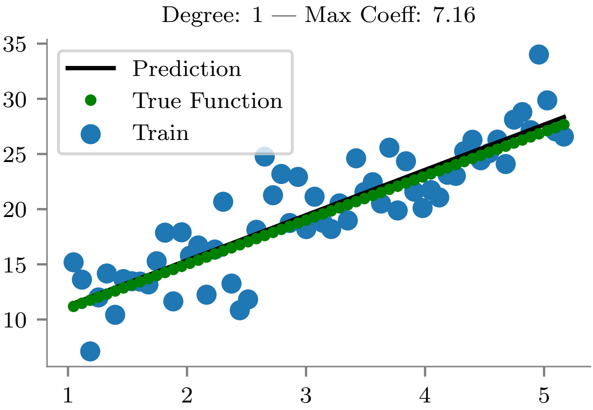


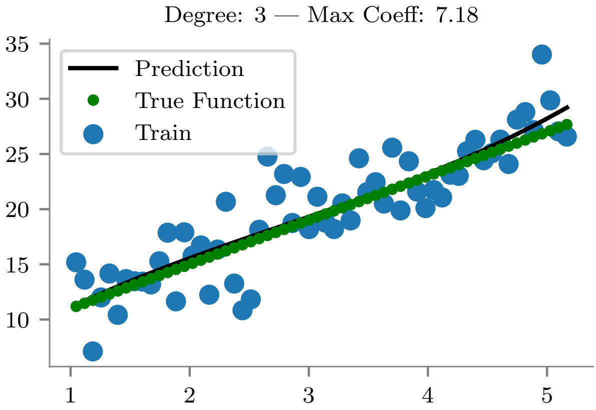
Base Data Set

Introduction



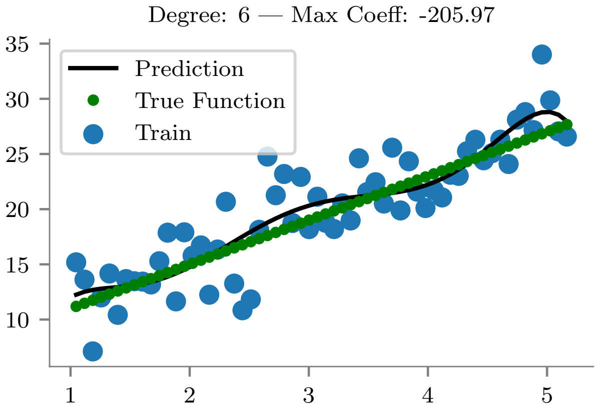
Fit with Degree 1

Introduction



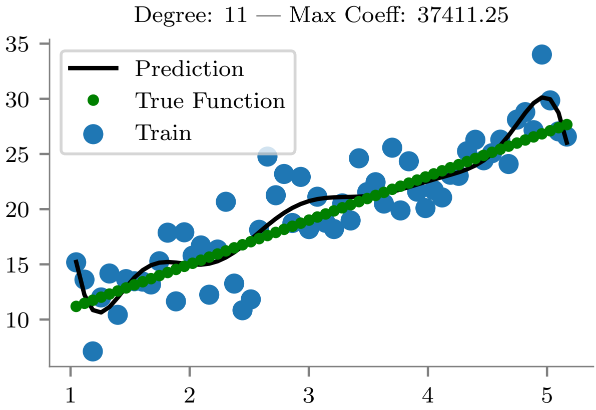
Fit with Degree 3

Introduction



Fit with Degree 6

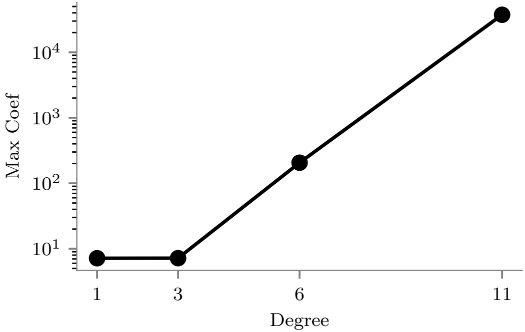
Introduction



Fit with Degree 11

Introduction

In the examples we notice that as the degree increases (as the prediction starts to overfit the base data), the maximum coefficient also increases.



Trend of the coefficients

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To prevent overfitting we place penalties on large θ_i

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Objective:

$$\text{Minimise } (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})$$
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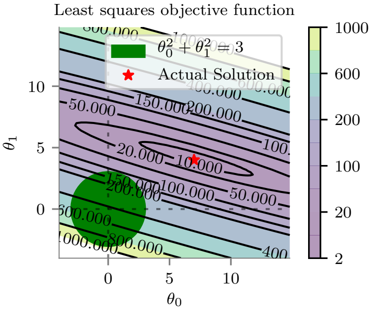
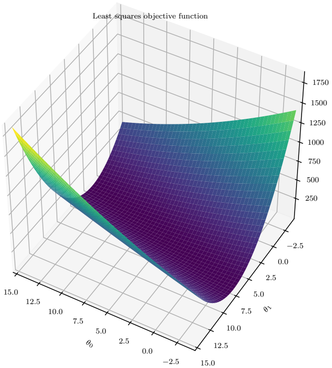
This is equivalent to

$$\text{Minimise } (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \delta^2 \boldsymbol{\theta}^T \boldsymbol{\theta}$$

Introduction



(a) Contour Plot



(b) Surface Plot

Visualization of the Example

KKT Conditions

To implement this we use KKT Conditions

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$$\text{s.t. } \boldsymbol{\theta}^T \boldsymbol{\theta} \leq S$$
$$L(\boldsymbol{\theta}, \mu) = (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \mu \left(\boldsymbol{\theta}^T \boldsymbol{\theta} - S \right)$$

where, $\mu \geq 0$ (and $\mu = \delta^2$)

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If $\mu = 0$
There is no
regularization
No effect on constraint

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where, $\mu \geq 0$ (and $\mu = \delta^2$)

If $\mu = 0$
There is no regularization
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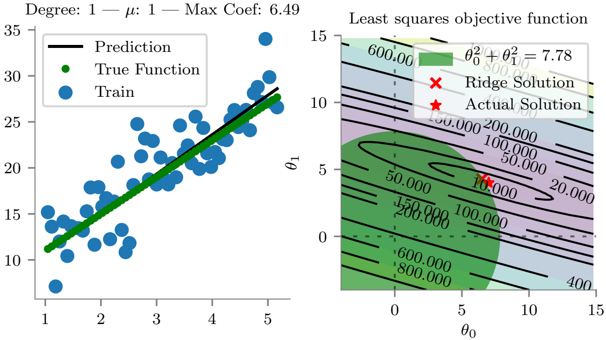
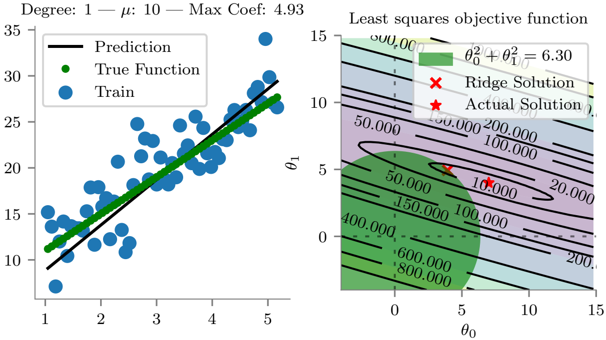
If $\mu \neq 0$
$\implies \boldsymbol{\theta}^T\boldsymbol{\theta} - S = 0$

Effect of μ



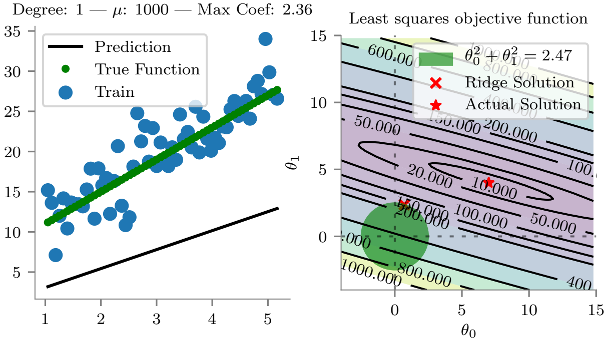
$\mu = 1$

Effect of μ



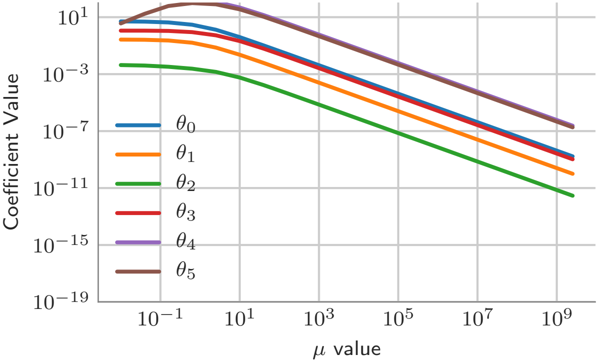
$\mu = 10$

Effect of μ



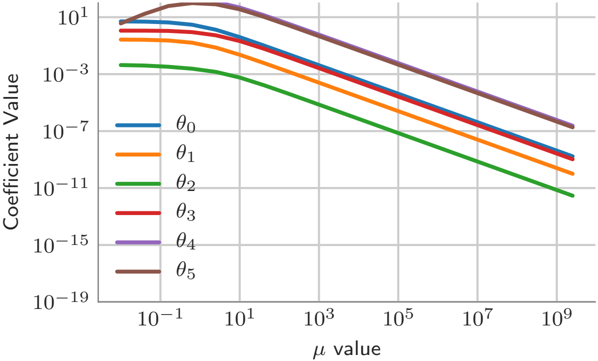
$$\mu = 1000$$

Effect of μ - Regularization of Parameters



Comparing the magnitudes of the coefficients with varying μ
(on the *Real Estate Data Set*)

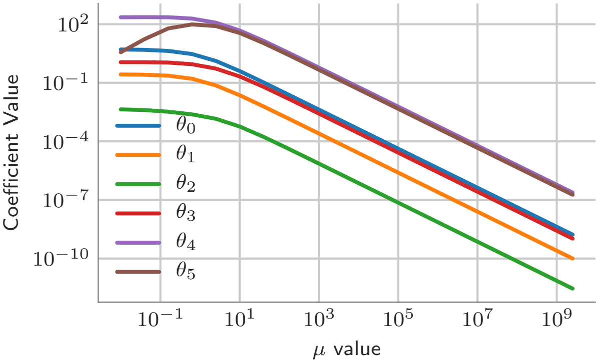
Effect of μ - Regularization of Parameters



Comparing the magnitudes of the coefficients with varying μ (on the *Real Estate Data Set*)

Are θ_i all zero for high μ?

Effect of μ - Regularization of Parameters



Comparing the magnitudes of the coefficients with varying μ
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Analytical Method

Ridge Objective:

$$\min_{\boldsymbol{\theta}} (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \mu \boldsymbol{\theta}^T \boldsymbol{\theta}$$

$$\begin{aligned}
\frac{\partial L(\boldsymbol{\theta}, \mu)}{\partial \boldsymbol{\theta}} &= 0 \\
\frac{\partial}{\partial \boldsymbol{\theta}} \left\{ \mathbf{y}^T \mathbf{y} - 2\mathbf{y}^T \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\theta}^T \mathbf{X}^T \mathbf{X}\boldsymbol{\theta} \right\} + \frac{\partial}{\partial \boldsymbol{\theta}} \mu \boldsymbol{\theta}^T \boldsymbol{\theta} &= 0 \\
\implies -\mathbf{X}^T \mathbf{y} + \left(\mathbf{X}^T \mathbf{X} + \mu \mathbf{I} \right) \boldsymbol{\theta} &= 0 \\
\implies \boldsymbol{\theta}^* &= \left(\mathbf{X}^T \mathbf{X} + \mu \mathbf{I} \right)^{-1} \mathbf{X}^T \mathbf{y}
\end{aligned}$$

Bias/Variance

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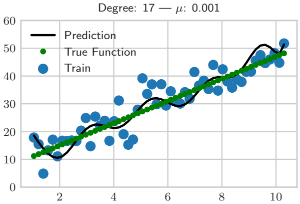

Fit High Order Polynomial
$\implies$ high variance
$\implies$ $\mu \to 0$

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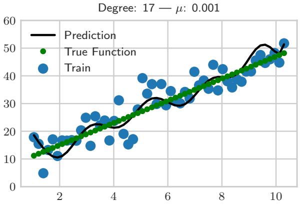

Fit High Order Polynomial
$\implies$ high variance
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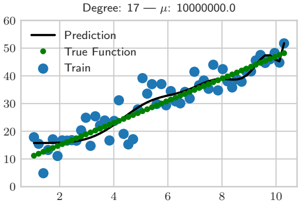


Fit High Order Polynomial
$\implies$ low variance
$\implies \mu \to \infty$

Example

Q.) Solve Regularized ($\mu = 2$) and Unregularized.

Example: Unregularised

$$\boldsymbol{\theta} = (\mathbf{X}^T\mathbf{X})^{-1}(\mathbf{X}^T\mathbf{y})$$

Example: Unregularised

$$\boldsymbol{\theta} = (\mathbf{X}^T\mathbf{X})^{-1}(\mathbf{X}^T\mathbf{y})$$

$$\mathbf{X}^T\mathbf{X} = \begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix}$$

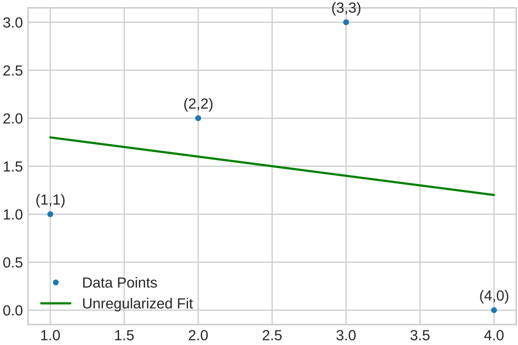
$$(\mathbf{X}^T\mathbf{X})^{-1} = \frac{1}{20}\begin{bmatrix} 30 & -10 \\ -10 & 4 \end{bmatrix}$$

$$\mathbf{X}^T\mathbf{y} = \begin{bmatrix} 6 \\ 14 \end{bmatrix}$$

Example: Unregularised

$$\boldsymbol{\theta} = (\mathbf{X}^T\mathbf{X})^{-1}(\mathbf{X}^T\mathbf{y})$$

$$\begin{bmatrix}\theta_0 \\ \theta_1\end{bmatrix} = \begin{bmatrix}2 \\ (-1/5)\end{bmatrix}$$



Example: Regularised

$$\boldsymbol{\theta} = (\mathbf{X}^T\mathbf{X} + \mu\mathbf{I})^{-1}(\mathbf{X}^T\mathbf{y})$$

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$$\boldsymbol{\theta} = (\mathbf{X}^T\mathbf{X} + \mu\mathbf{I})^{-1}(\mathbf{X}^T\mathbf{y})$$

$$\mathbf{X}^T\mathbf{X} = \begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix}$$

$$\mathbf{X}^T\mathbf{X} + \mu\mathbf{I} = \begin{bmatrix} 6 & 10 \\ 10 & 32 \end{bmatrix}$$

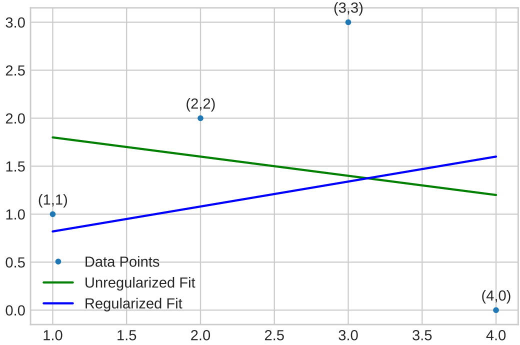
$$(\mathbf{X}^T\mathbf{X} + \mu\mathbf{I})^{-1} = \frac{1}{92}\begin{bmatrix} 32 & -10 \\ -10 & 6 \end{bmatrix}$$

$$\mathbf{X}^T\mathbf{y} = \begin{bmatrix} 6 \\ 14 \end{bmatrix}$$

Example: Regularised

$$\boldsymbol{\theta} = (\mathbf{X}^T\mathbf{X} + \mu\mathbf{I})^{-1}(\mathbf{X}^T\mathbf{y})$$

$$\begin{bmatrix}\theta_0 \\ \theta_1\end{bmatrix} = \begin{bmatrix}0.56 \\ 0.26\end{bmatrix}$$



Multi-collinearity

$(\mathbf{X}^T\mathbf{X})^{-1}$ is not computable when $|\mathbf{X}^T\mathbf{X}| = 0$.
This was a drawback of using linear regression

$$\mathbf{X} = \begin{bmatrix} 1 & 1 & 2 \\ 1 & 2 & 4 \\ 1 & 3 & 6 \end{bmatrix}$$

The matrix $\mathbf{X}$ is not full rank.

Multi-collinearity

But with ridge regression, the matrix to be inverted is $\mathbf{X}^T\mathbf{X} + \mu\mathbf{I}$ and not $\mathbf{X}^T\mathbf{X}$.

$$\mathbf{X}^T\mathbf{X} + \mu\mathbf{I} = \begin{bmatrix} 3+\mu & 6 & 12 \\ 6 & 14+\mu & 28 \\ 12 & 28 & 56+\mu \end{bmatrix}$$

The matrix $\mathbf{X}^T\mathbf{X}$ would be full rank for $\mu > 0$.

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The matrix $\mathbf{X}^T\mathbf{X}$ would be full rank for $\mu > 0$.
Another interpretation of “regularisation”

Extension of the analytical model

For ridge with no penalty on θ_0

$$\hat{\boldsymbol{\theta}} = \left(\mathbf{X}^T\mathbf{X} + \mu\mathbf{I}^*\right)^{-1}\mathbf{X}^T\mathbf{y}$$

where,

$$\mathbf{I}^* = \begin{bmatrix} {\color{red}0} & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix}$$

Ridge Solution using Gradient Descent

- $\boldsymbol{\theta} = \boldsymbol{\theta} - \alpha \frac{\partial}{\partial \boldsymbol{\theta}} ((\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \mu \boldsymbol{\theta}^\top \boldsymbol{\theta})$

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- $\boldsymbol{\theta} = \boldsymbol{\theta} - \alpha(-2\mathbf{X}^\top \mathbf{y} + 2\mathbf{X}^\top \mathbf{X}\boldsymbol{\theta} + 2\mu \mathbf{I}\boldsymbol{\theta})$

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- $\boldsymbol{\theta} = (1 - 2\alpha\mu\mathbf{I})\boldsymbol{\theta} - \alpha(-2\mathbf{X}^\top \mathbf{y} + 2\mathbf{X}^\top \mathbf{X}\boldsymbol{\theta})$

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- $\boldsymbol{\theta} = \underbrace{(1 - 2\alpha\mu\mathbf{I})\boldsymbol{\theta}}_{\text{Shrinking } \boldsymbol{\theta}} - \alpha(-2\mathbf{X}^\top \mathbf{y} + 2\mathbf{X}^\top \mathbf{X}\boldsymbol{\theta})$

Ridge Solution using Gradient Descent

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- Contrast with update equation for unregularised regression:

Ridge Solution using Gradient Descent

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- Contrast with update equation for unregularised regression:
- $\boldsymbol{\theta} = \underbrace{\boldsymbol{\theta}}_{\text{No Shrinking } \boldsymbol{\theta}} - \alpha(-2\mathbf{X}^\top \mathbf{y} + 2\mathbf{X}^\top \mathbf{X}\boldsymbol{\theta})$